# The Transformer architecture

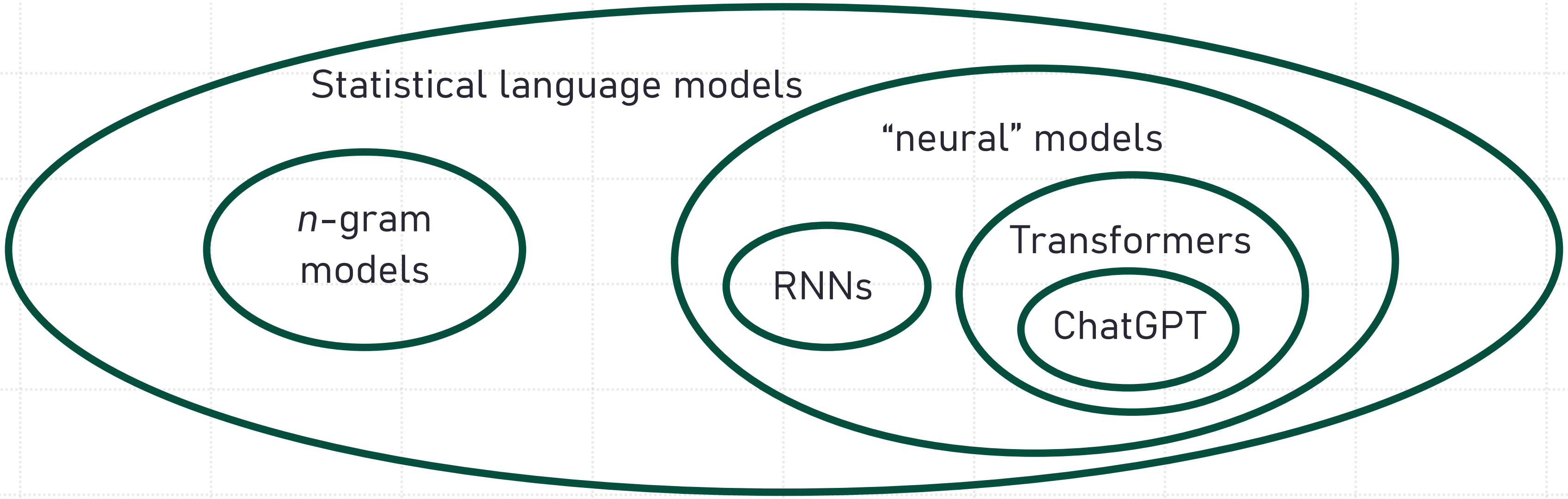
*COGS 150*

*Sean Trott*

*Winter 2024*

# A brief taxonomy

- Many approaches to **language modeling**.
- All revolve around **statistical learning** in some way.



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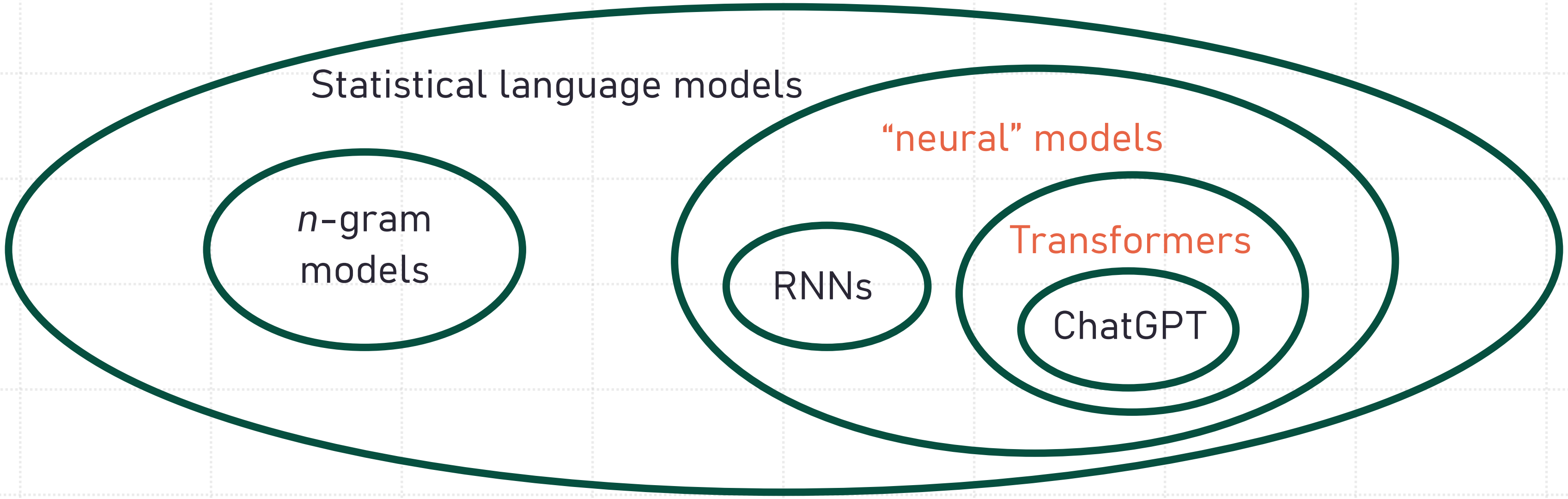

# Lecture plan

- “Attention”: high-level introduction and motivation.
- The transformer architecture—is attention all you need?
- The advent of “pre-trained LLMs”.

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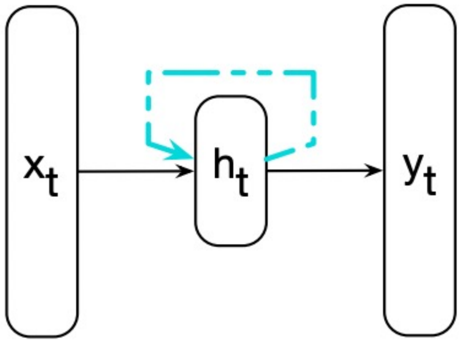
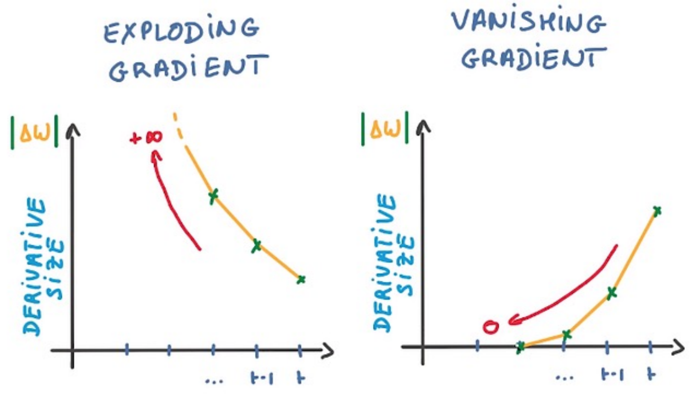



# RNNs: recap, and limitations

- A **recurrent neural network (RNN)** has at least one *recurrent* connection, which acts as a kind of "memory" of the context.
- RNNs work pretty well, but do have limitations.

**Limitation #1**:
Vanishing/exploding gradient.




**Limitation #2**:
Training is hard to parallelize.

Recurrent structure makes it hard to process many batches in parallel—harder to take advantage of compute.

# The advent of “attention”

**Attention** is a mechanism that—metaphorically—allows an LLM to “focus” (or “attend”) on specific elements in a sequence.

- Often, <u>accurate predictions</u> depend on words from a while ago.

Check the program log and find out whether it ran please.

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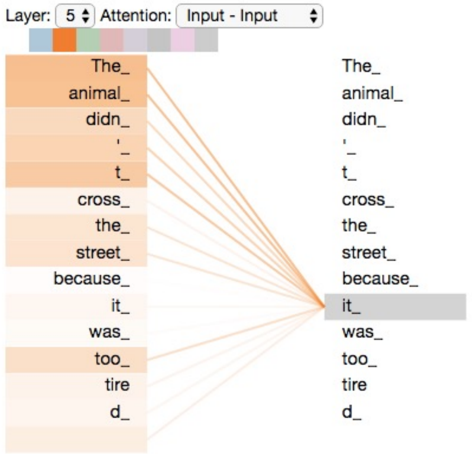
- This also helps identify relationships between elements in the sequence.

The animal didn’t cross the street because it was tired.



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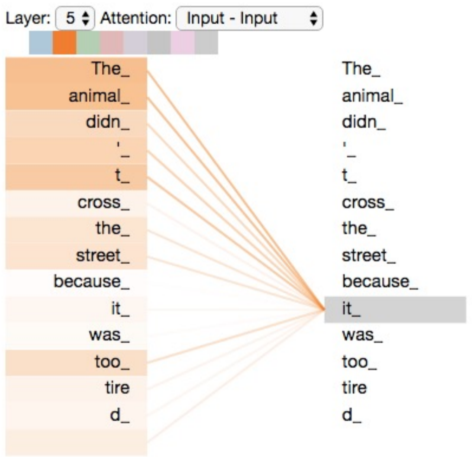

But how does this actually <u>work</u>?

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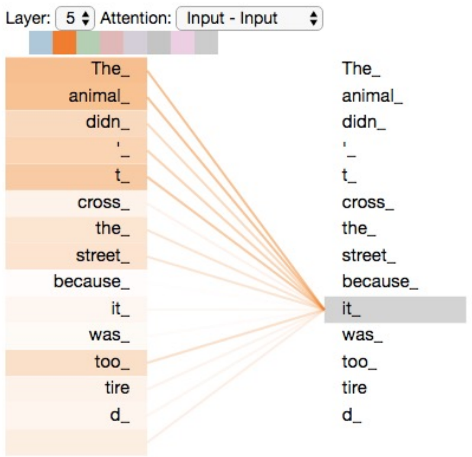
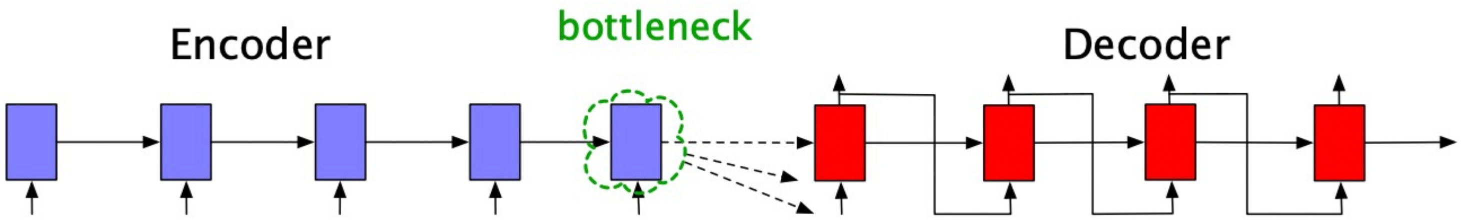


# Attention: the origins

- Originally, attention was developed to help with **machine translation**.
- Traditional, RNN-based translation models had a “bottleneck” in their design.

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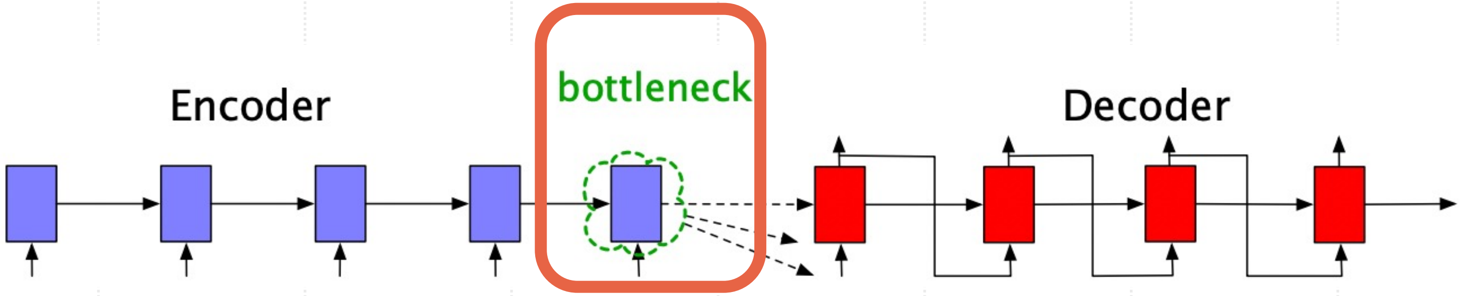


Encodes source language.

Decodes to target language.

**Bottleneck**: *all* the information required to translate a sentence must be packed into this last hidden state.

# Attention: the origins

- Originally, attention was developed to help with **machine translation**.
- Traditional, RNN-based translation models had a “bottleneck” in their design.
- Attention is a mechanism for putting *all* those hidden states into a single fixed-length vector—by focusing on what’s most relevant.

**Dot-product attention**: implements “relevance” as *embedding similarity.*

To illustrate this, let’s look at an example from a domain we’re already familiar with—language modeling.

# Dot-product attention: illustrated

In **dot-product attention**, the dot product between every pair of words is used to build a custom, context-dependent vector.

The cat sat on ___

"on"

The

cat

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|---|---|
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Each of these is represented by an **embedding**.

The dot product captures the **similarity** in embeddings.

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The cat sat on ___

| | | "on" | $w * c$ |
|---|---|---|---|
| V1 | The | | .2 |
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Numbers made up for illustration purposes!

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The cat sat on ___

| | | "on" | $w * c$ | $\sigma(x)_j = \frac{e^{x_j}}{\sum_k e^{x_k}}$ |
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| V1 | The | | .2 | .2 |
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Now, we **soft-max** these values to create a probability distribution.

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These are our **attention weights**.

Each represents the "relevance" of $V_n$ to "on".

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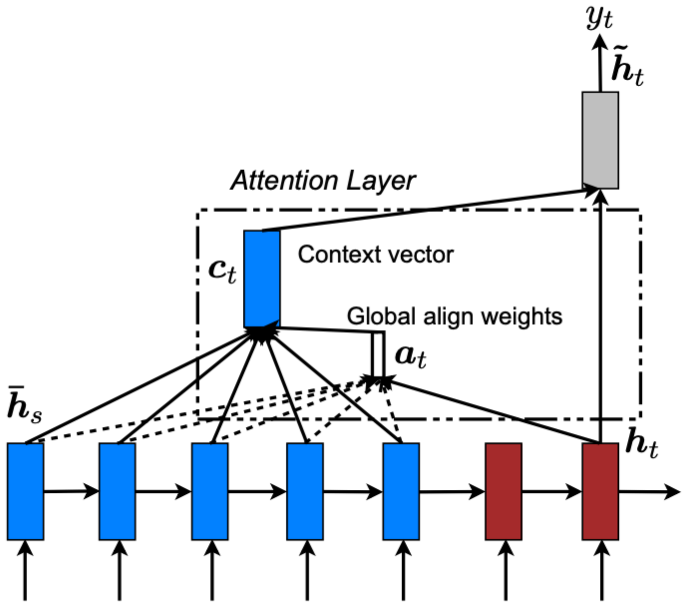


Now, compute **weighted average** over all hidden states—using these attention scores as "weights"!

$$\mathbf{c}_i = \sum_j \alpha_{ij}\, \mathbf{h}^e_j$$

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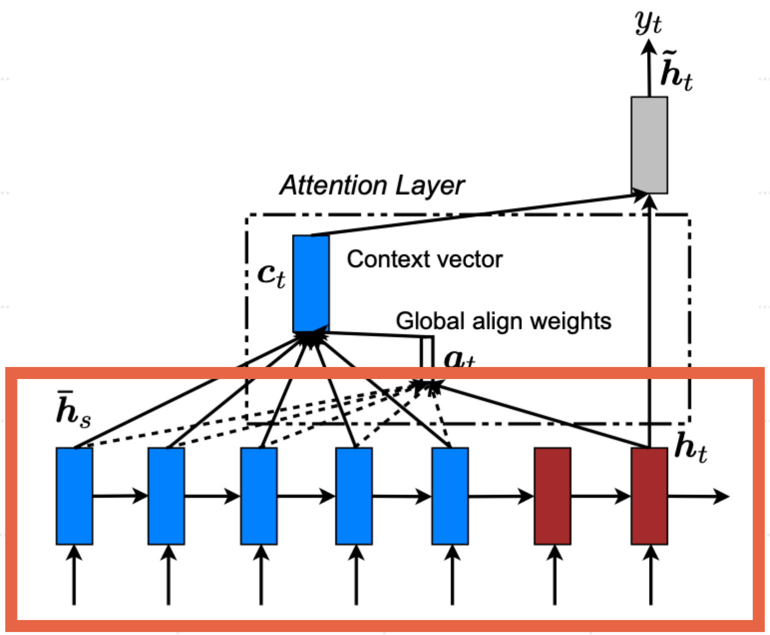
Hidden states

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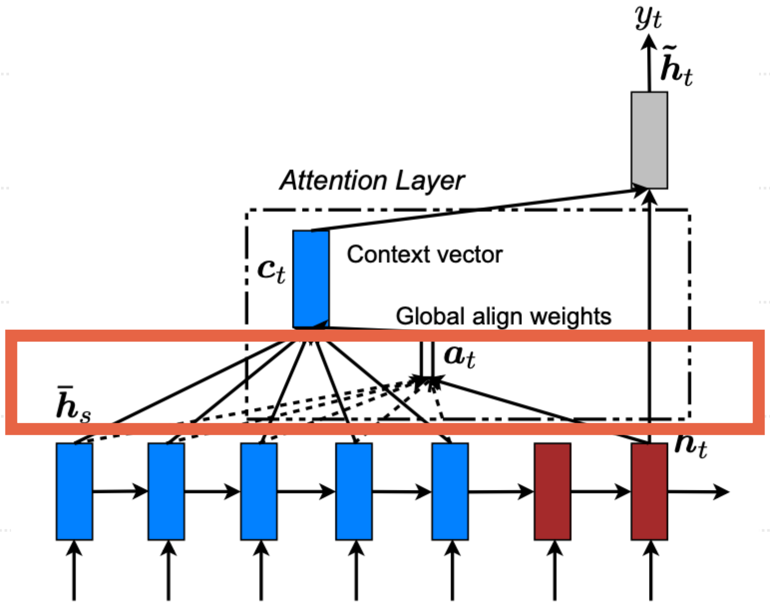
Compute attention weights

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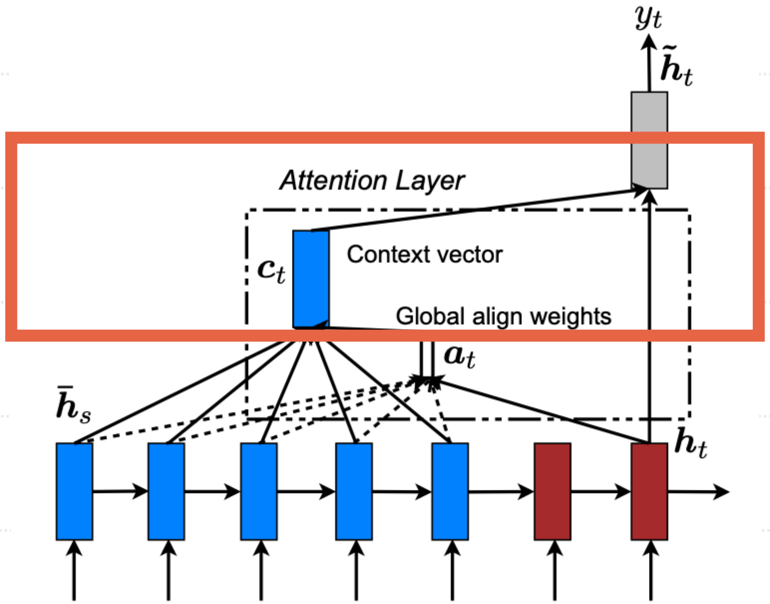
# Dot-product attention: illustrated

In **dot-product attention**, the dot product between every pair of words is used to build a custom, context-dependent vector.

Use attention weights to create new **context vector**.

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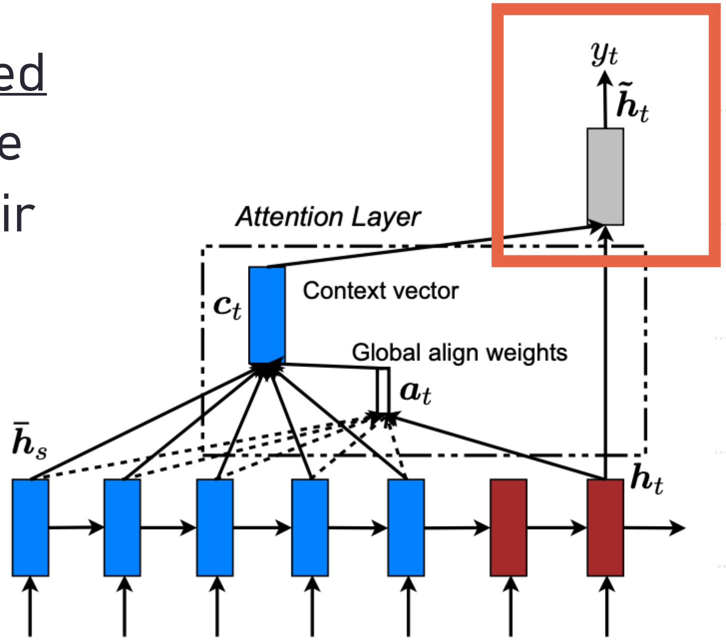
Predictions are now <u>weighted</u> by different elements of the sequence depending on their "relevance".

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In **dot-product attention**, the dot product between every pair of words is used to build a custom, context-dependent vector.

In theory, we can do this at each layer of a neural network.

But the dot product is still a pretty coarse measure of attention.

Can we do better?

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- The transformer architecture—is attention all you need?
- The advent of “pre-trained LLMs”.

"RNN + Attention—but throw out the RNN!"

# Introducing transformers

The **Transformer** is a neural network architecture that uses multi-head self-attention, with no recurrent units.

- Use a **fixed context window**.
- No **recurrent connections**.
- Use **self-attention**.
- Have multiple attention "heads" (**multi-head self-attention**).
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What do these aspects of a transformer remind you of?

A traditional **feed-forward neural language model**!

(Note: this is why you often hear about the "context window size" of models like ChatGPT, Claude, etc.)

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These are new concepts—let's focus on **self-attention** first.

# Self-attention: match-making for words

In **self-attention**, the relevance of each word to each other is calculated in context and shared, informing the model's predictions.

**Query (Q)**: representation of current word, used to score against all other words in sequence.

**Key (K)**: labels for other words in sequence, which we "match" against in our search.

**Value (V)**: represent the "content" of each word, which are weighed by attention scores.

A robot must obey the orders given it…

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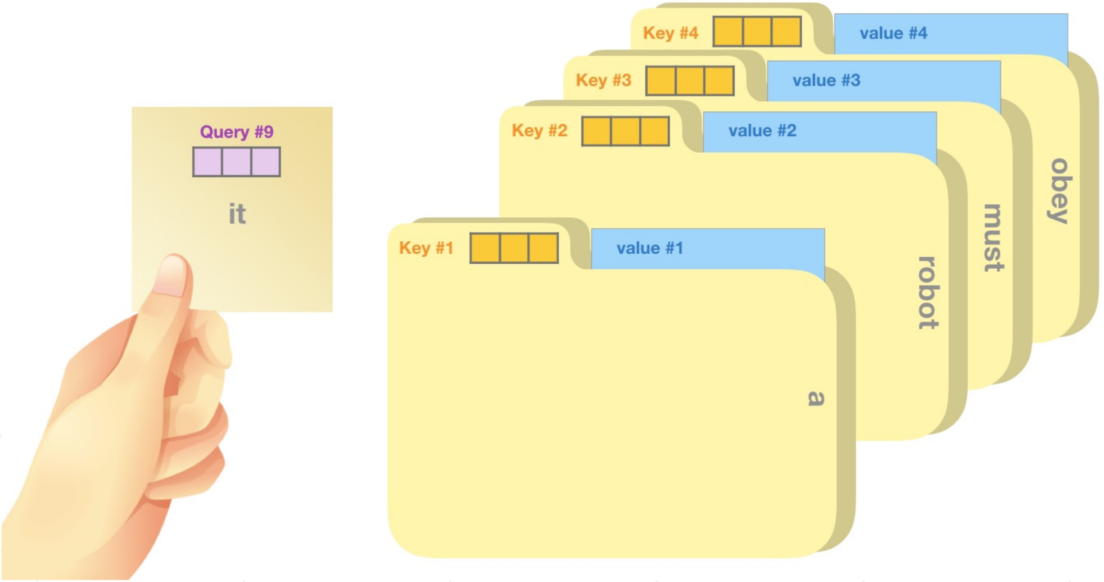

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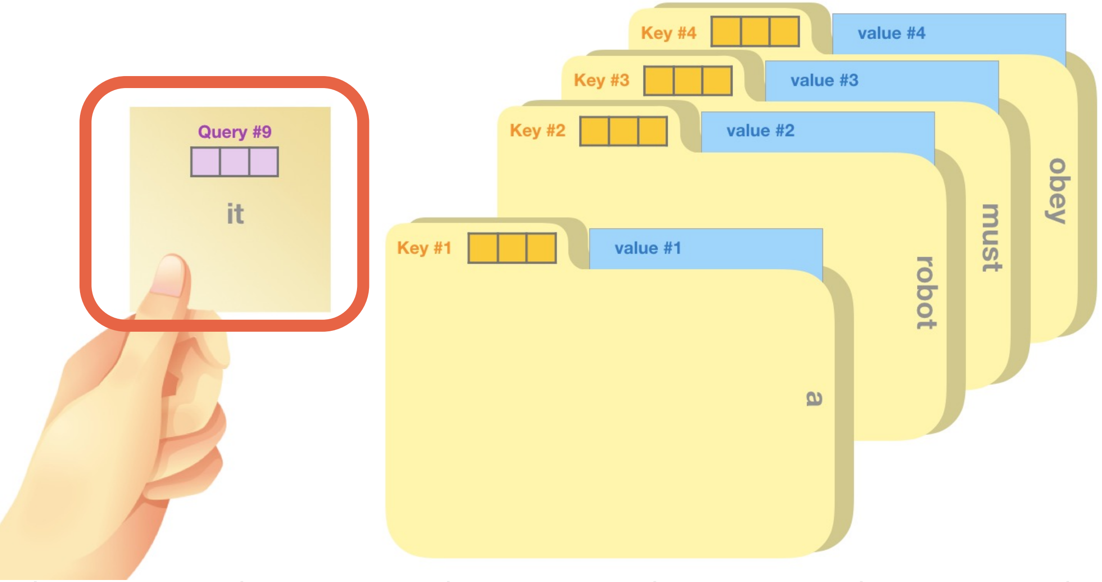

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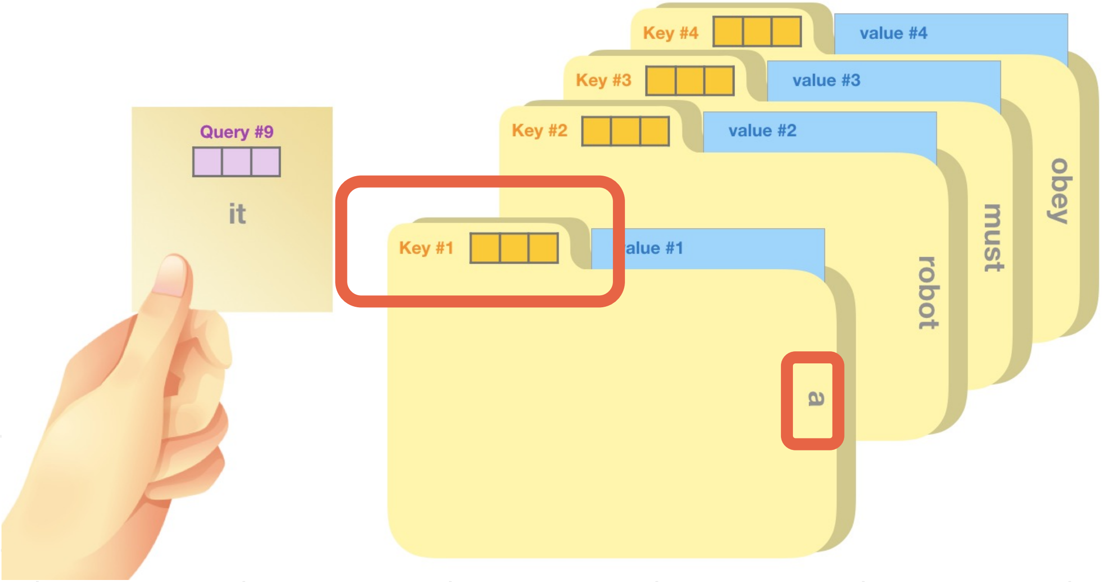

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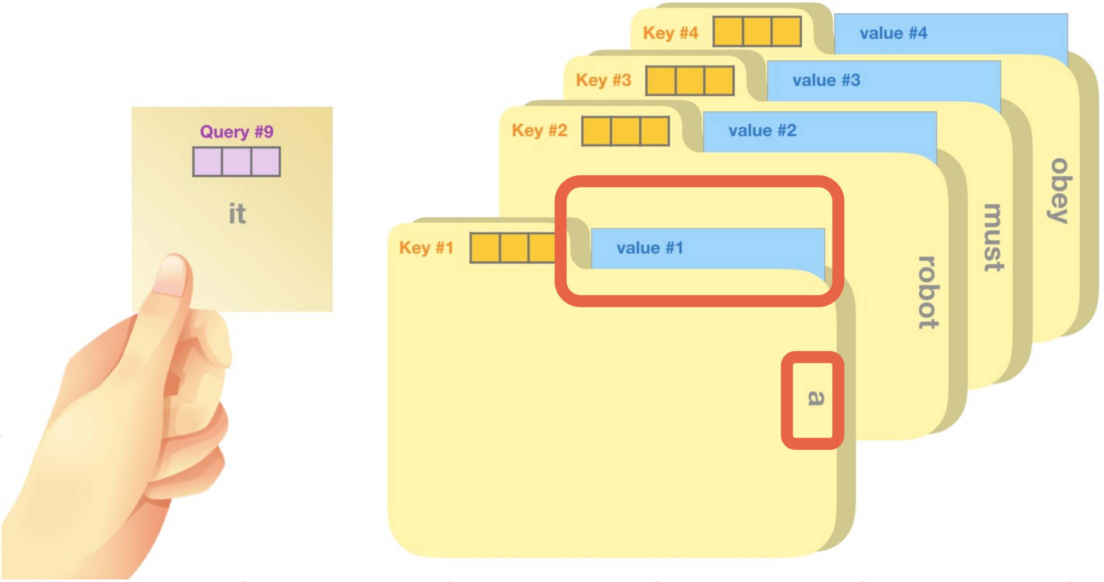

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To compute **attention score**, multiply query by key vectors for each pair.

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{q}_i \cdot \mathbf{k}_j$$

(We then **normalize** and **soft-max** these scores to get a probability distribution.)

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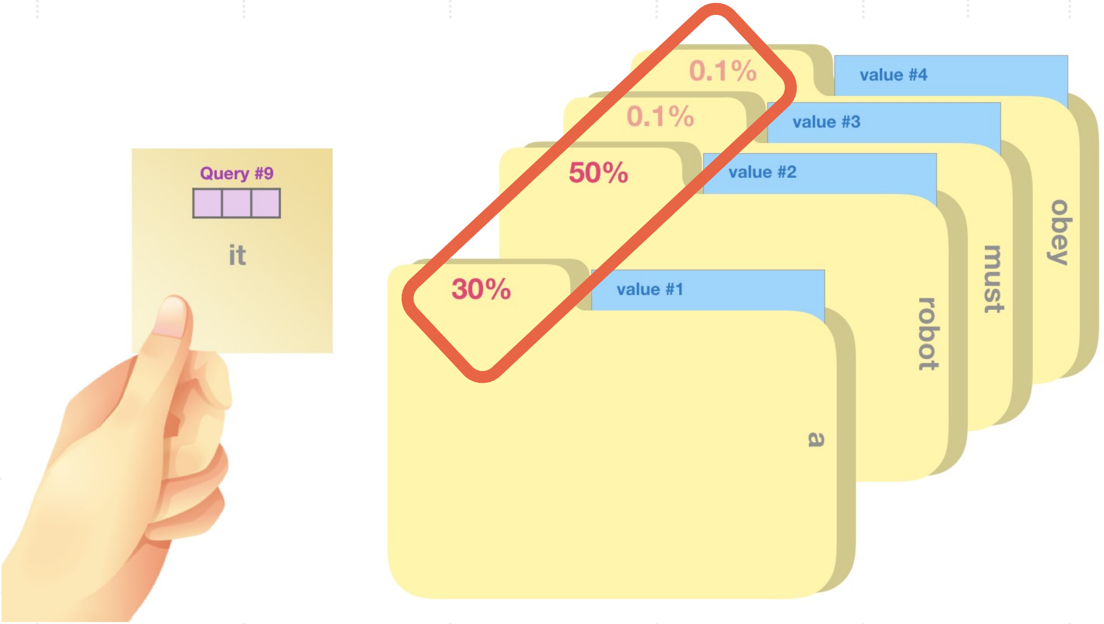

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Now, multiply (and sum) attention scores by value vectors.

$$\mathbf{y}_i = \sum_{j \le i} \alpha_{ij} \mathbf{v}_j$$

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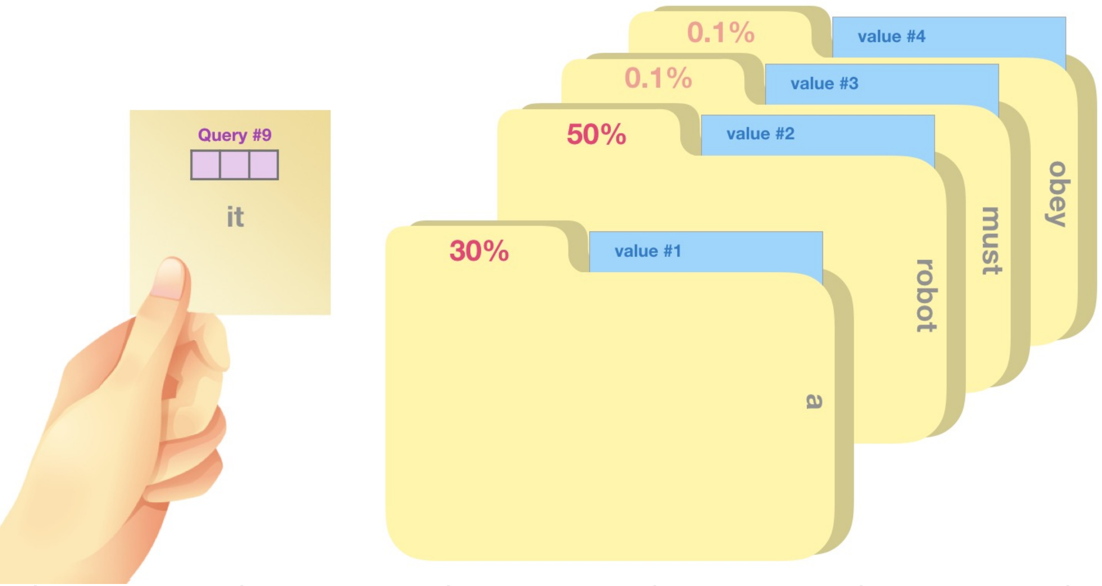

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| Word | Value vector | Score | Value X Score |
|---|---|---|---|
| <s> | | 0.001 | |
| a | | 0.3 | |
| robot | | 0.5 | |
| must | | 0.002 | |
| obey | | 0.001 | |
| the | | 0.0003 | |
| orders | | 0.005 | |
| given | | 0.002 | |
| | | 0.19 | |
| | | Sum: | |

This is our new **contextualized embedding** for "it".

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# Self-attention: match-making for words

In **self-attention**, the relevance of each word to each other is calculated in context and shared, informing the model's predictions.

We compute **attention scores** between each word $w_t$ and every word that comes before it.

In an **auto-regressive model**, we prevent attention from "looking ahead" at future words.

N

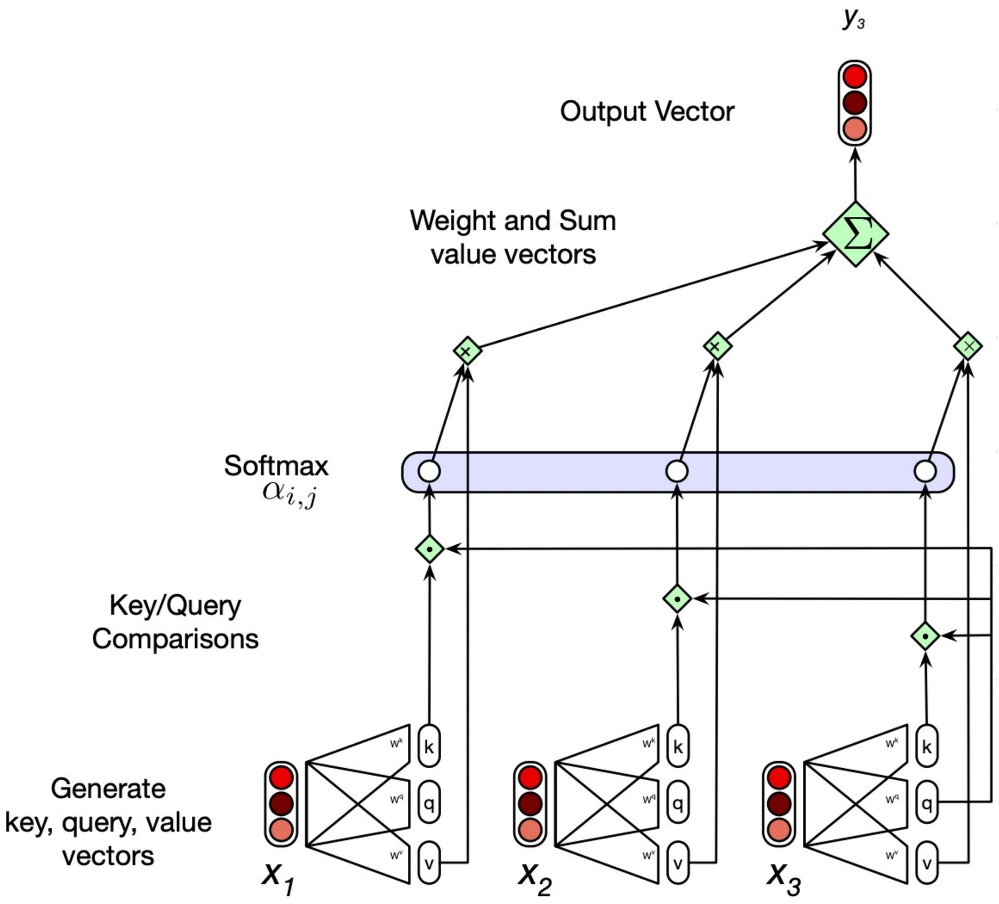
| | | | | |
|---|---|---|---|---|
| q1•k1 | −∞ | −∞ | −∞ | −∞ |
| q2•k1 | q2•k2 | −∞ | −∞ | −∞ |
| q3•k1 | q3•k2 | q3•k3 | −∞ | −∞ |
| q4•k1 | q4•k2 | q4•k3 | q4•k4 | −∞ |
| q5•k1 | q5•k2 | q5•k3 | q5•k4 | q5•k5 |

N

In terms of compute time, how "efficient" is this process?

It's **quadratic**—we must compute dot product between every pair of tokens in the input.

# Self-attention: a closer look




Suppose we are computing **self-attention** for $X_3$.

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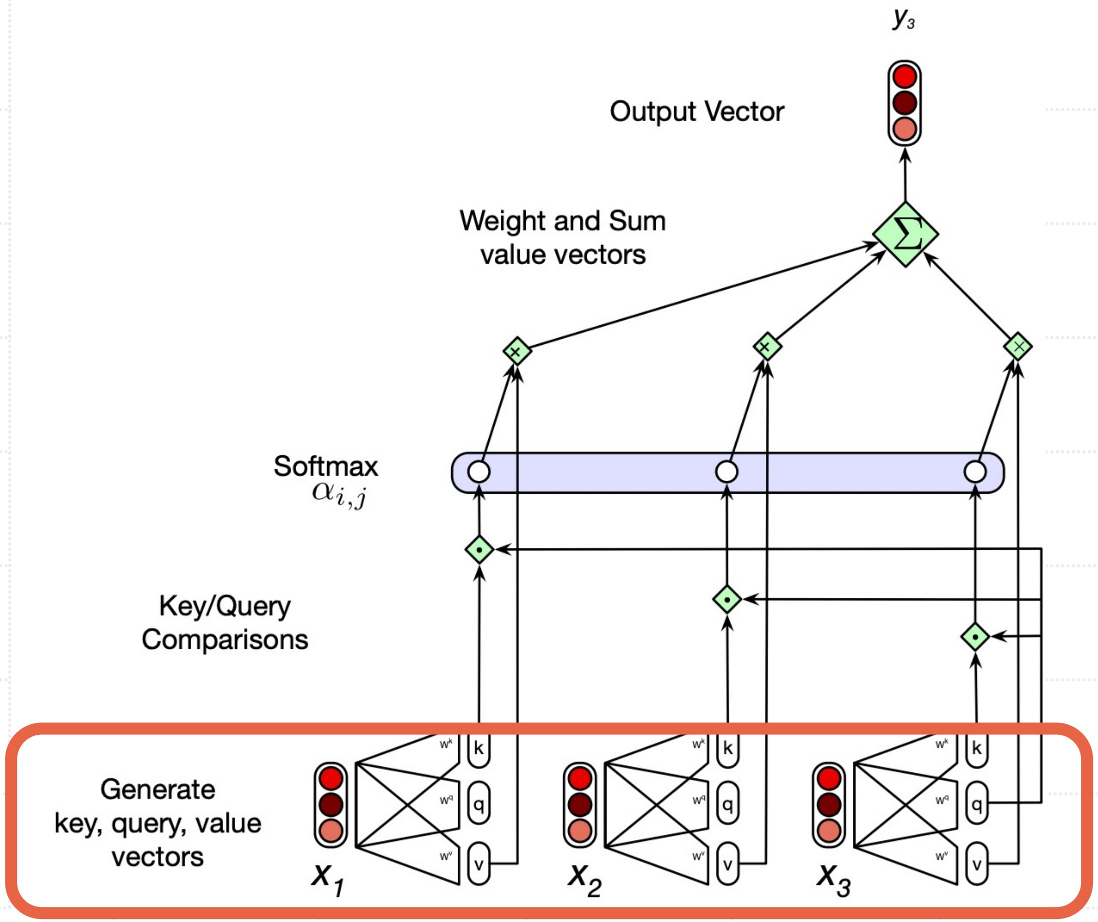


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For each word in sequence, compute **key**, **query**, and **value** vectors.

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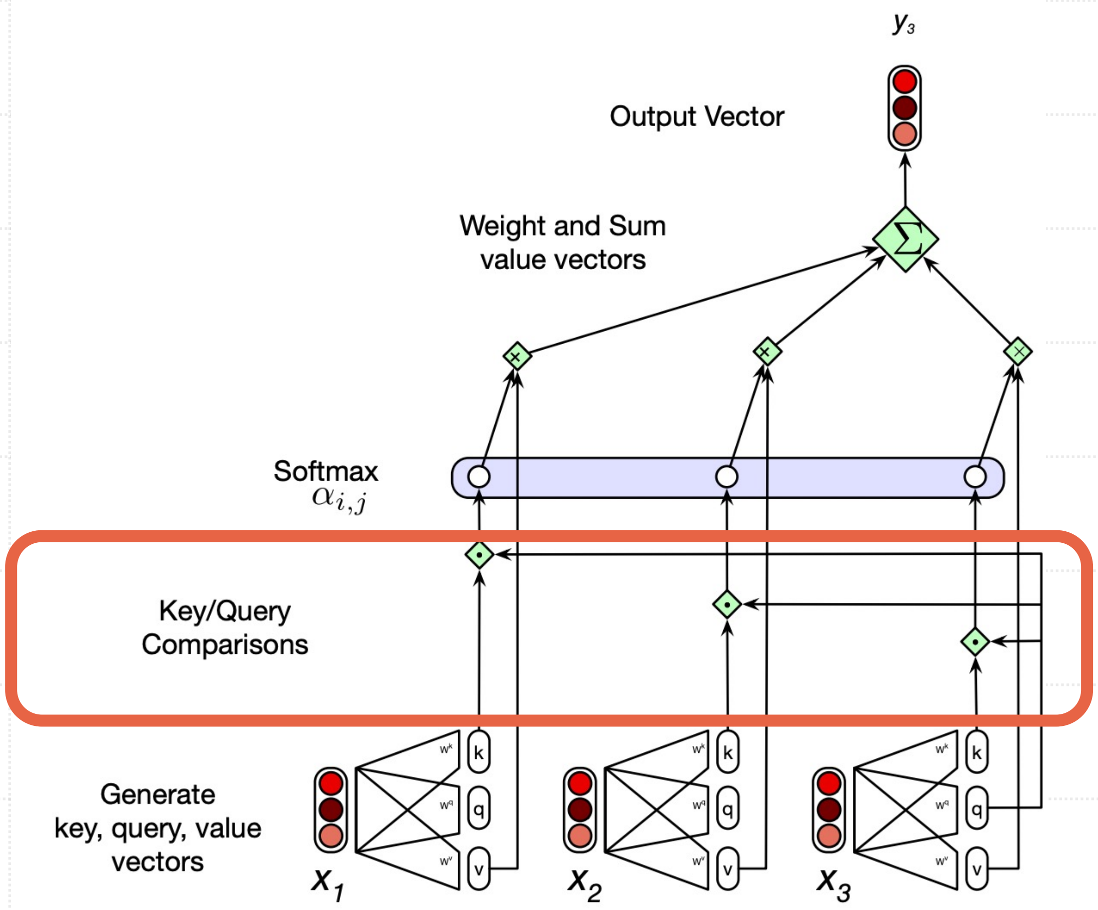


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Compute relevance of $X_1$ and $X_2$ to $X_3$.

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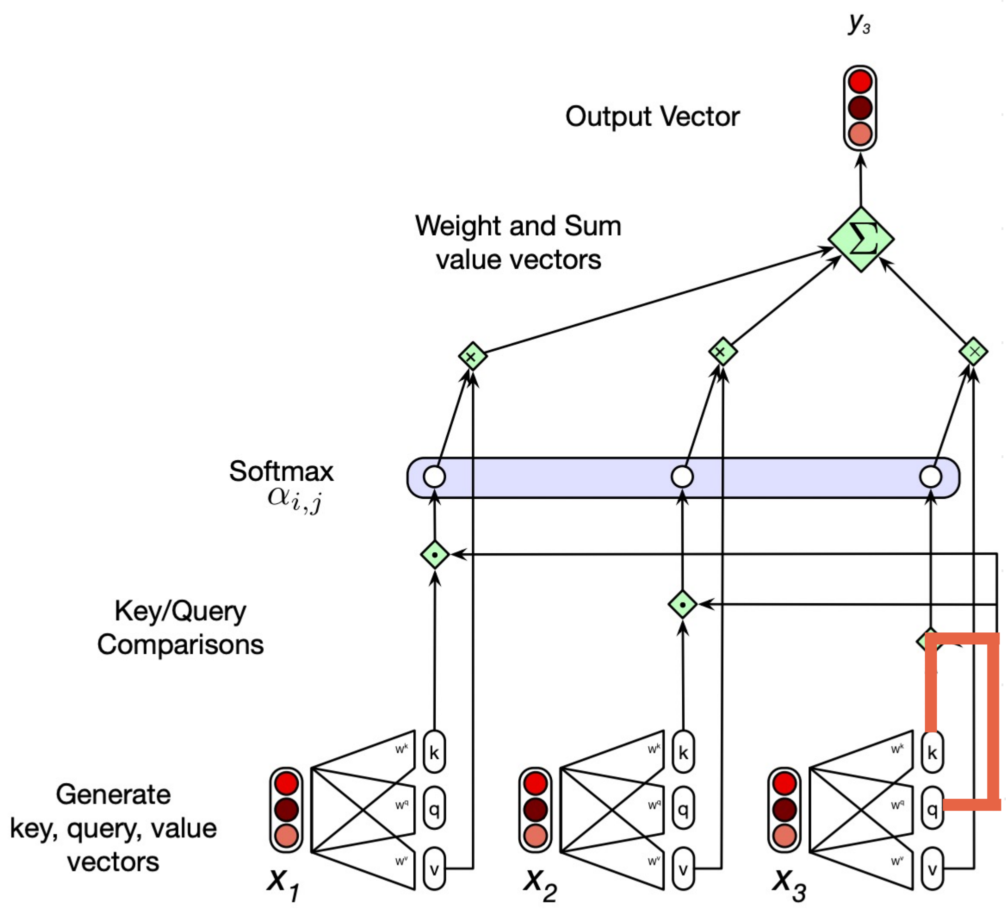


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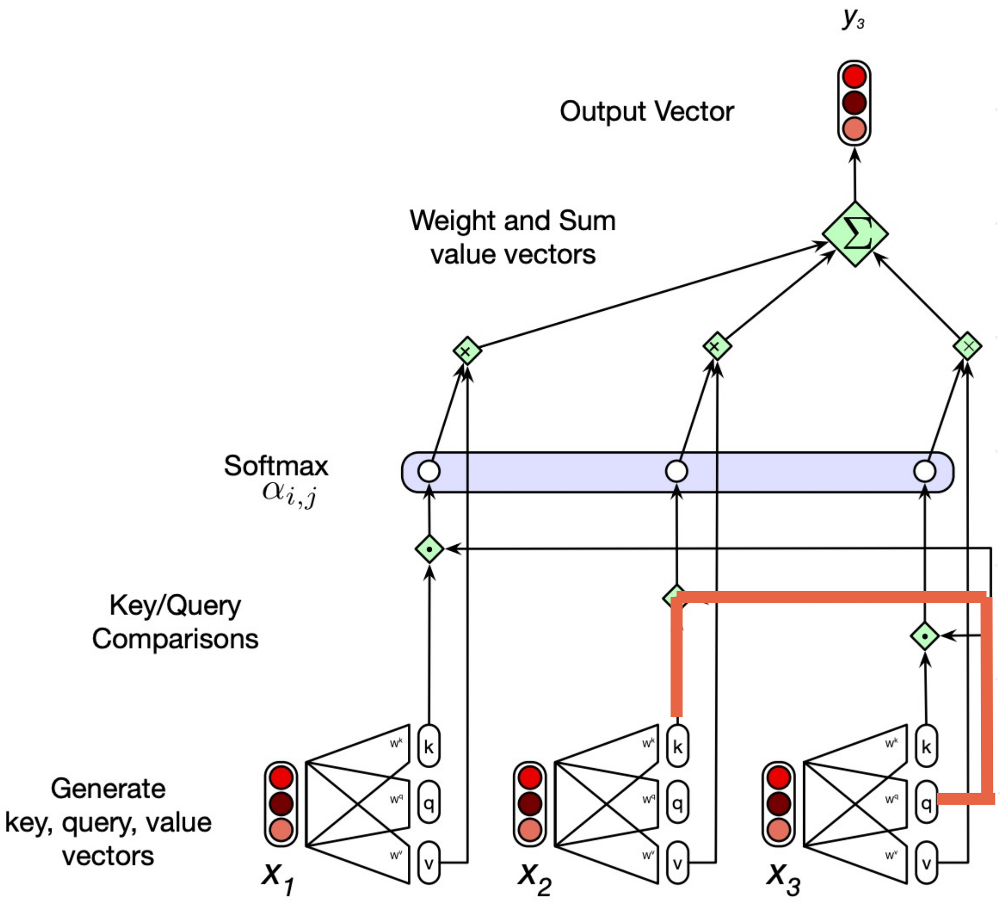


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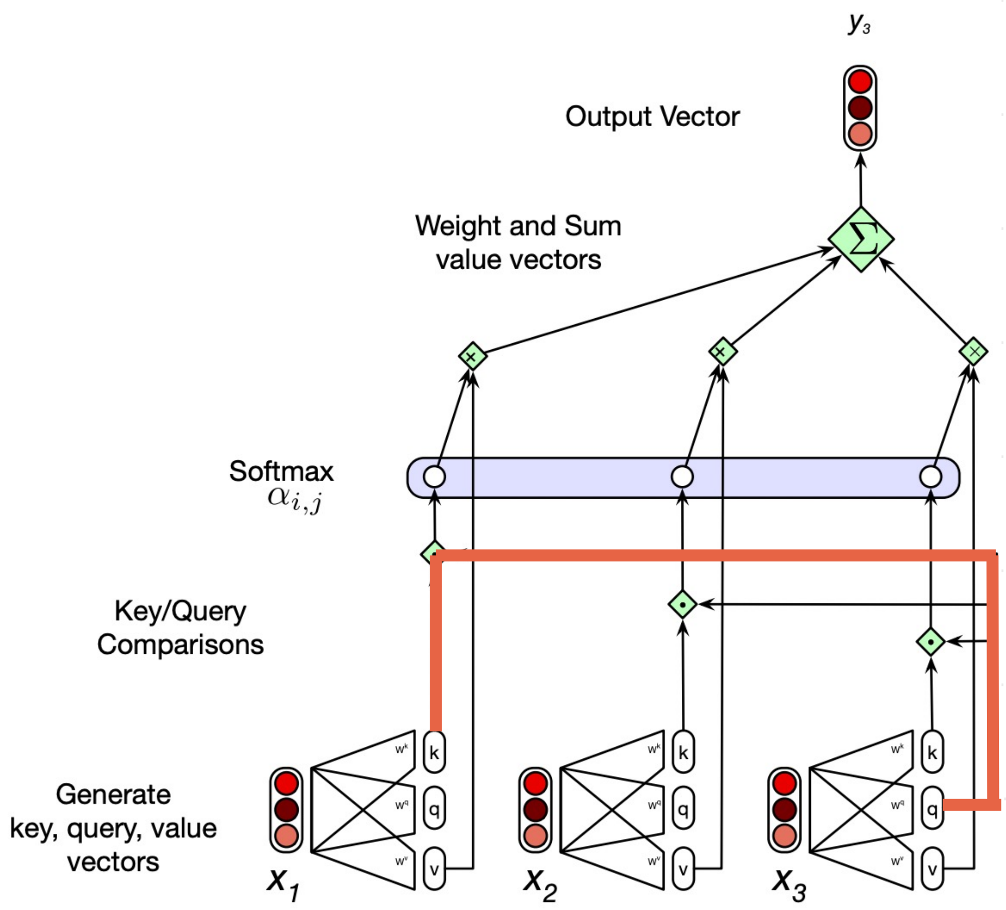


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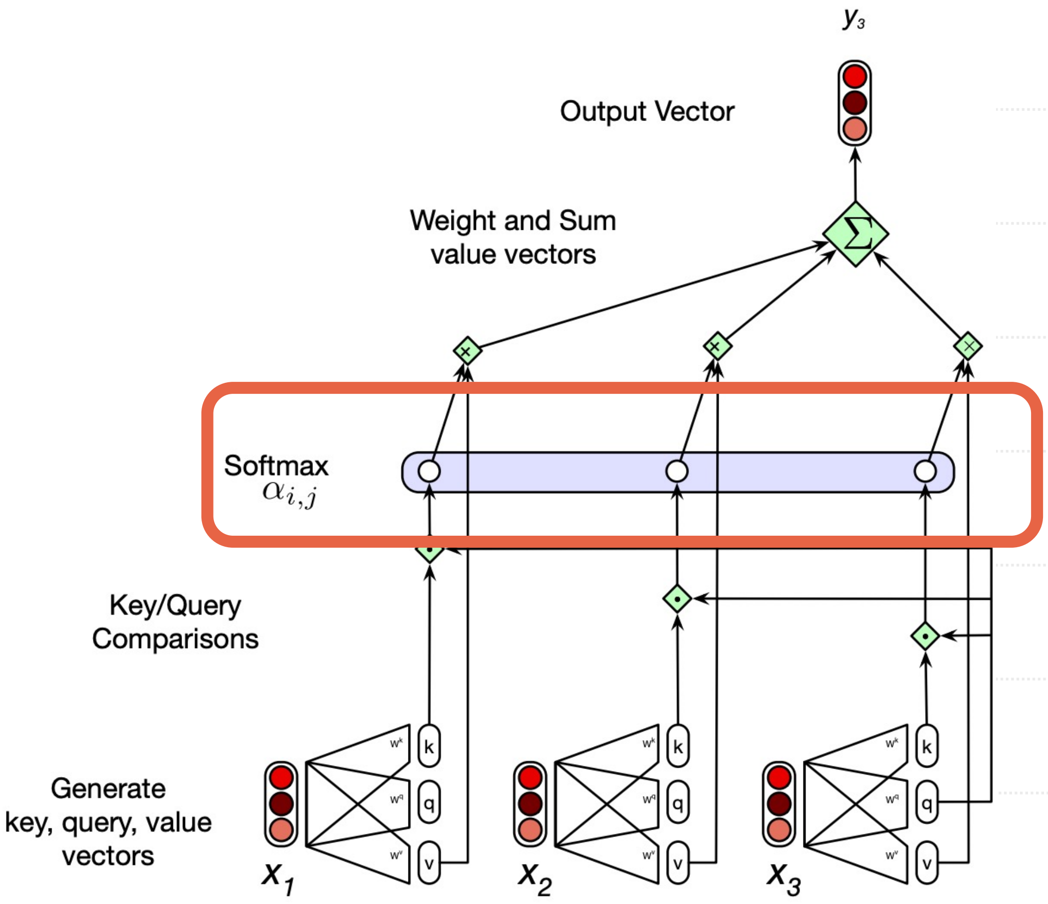


Suppose we are computing **self-attention** for $X_3$.

Soft-max these to get **attention scores**.

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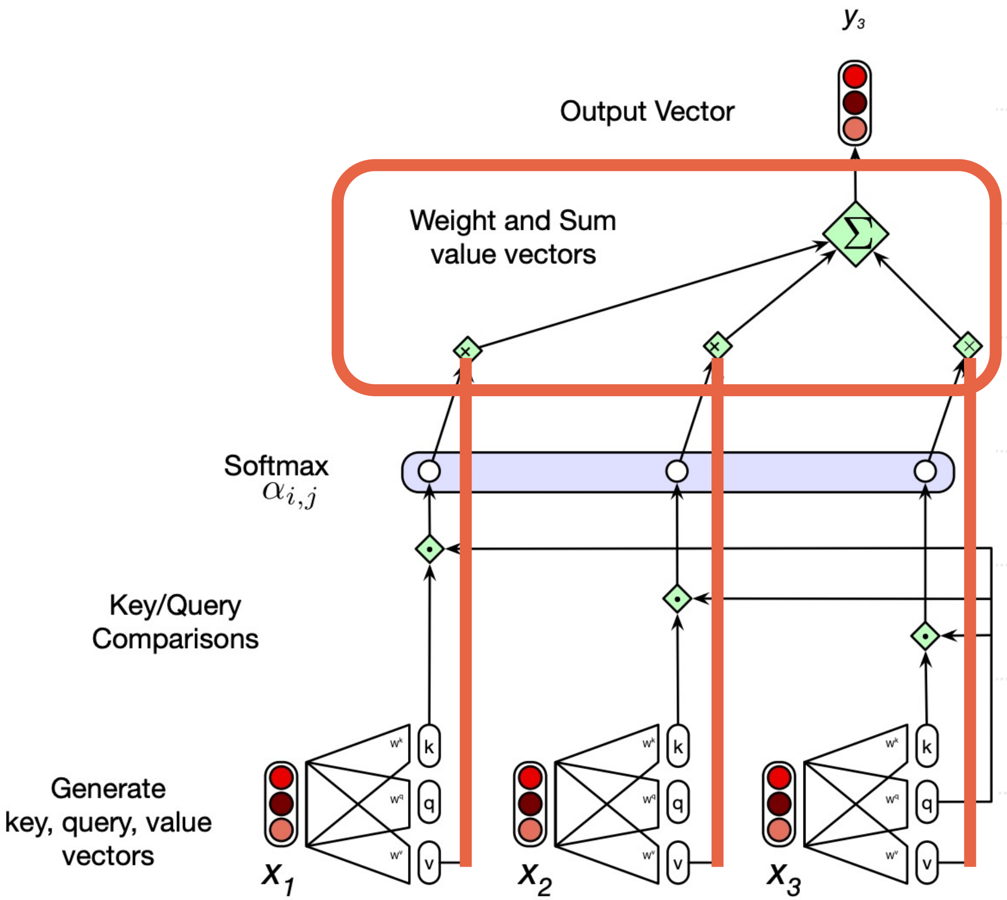


Suppose we are computing **self-attention** for $X_3$.

Use attention scores to weigh the **value vectors**.

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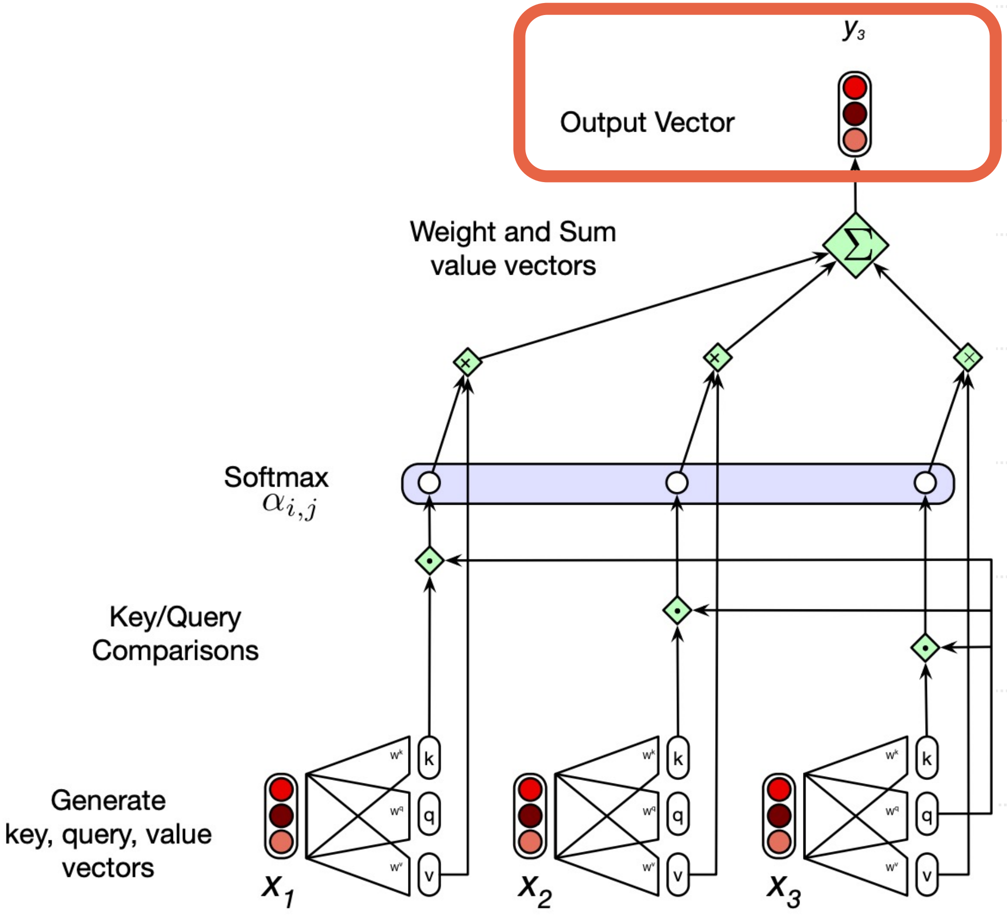
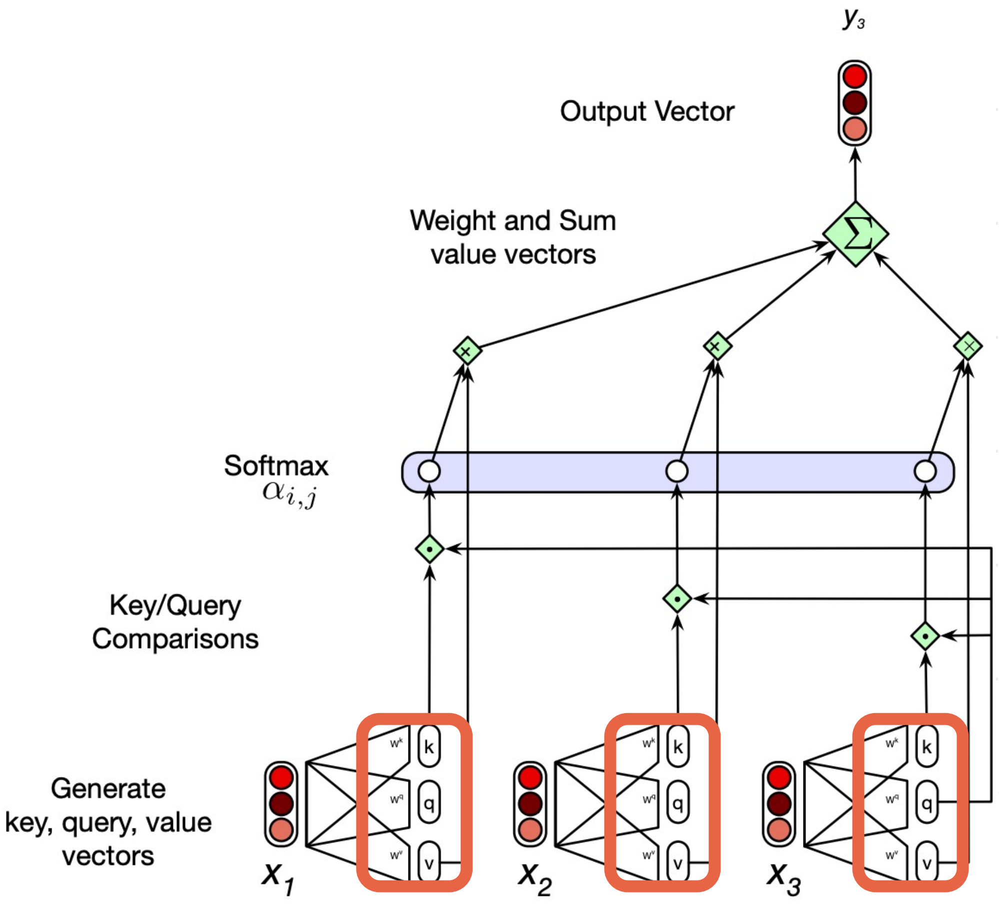



Suppose we are computing **self-attention** for $X_3$.

The result is a new embedding $Y_3$, which "folds in" the relevant information from $X_1$ and $X_2$ into $X_3$.

https://jalammar.github.io/illustrated-gpt2/#part-1-got-and-language-modeling

# Self-attention: a closer look




Where do Q, K, V come from?

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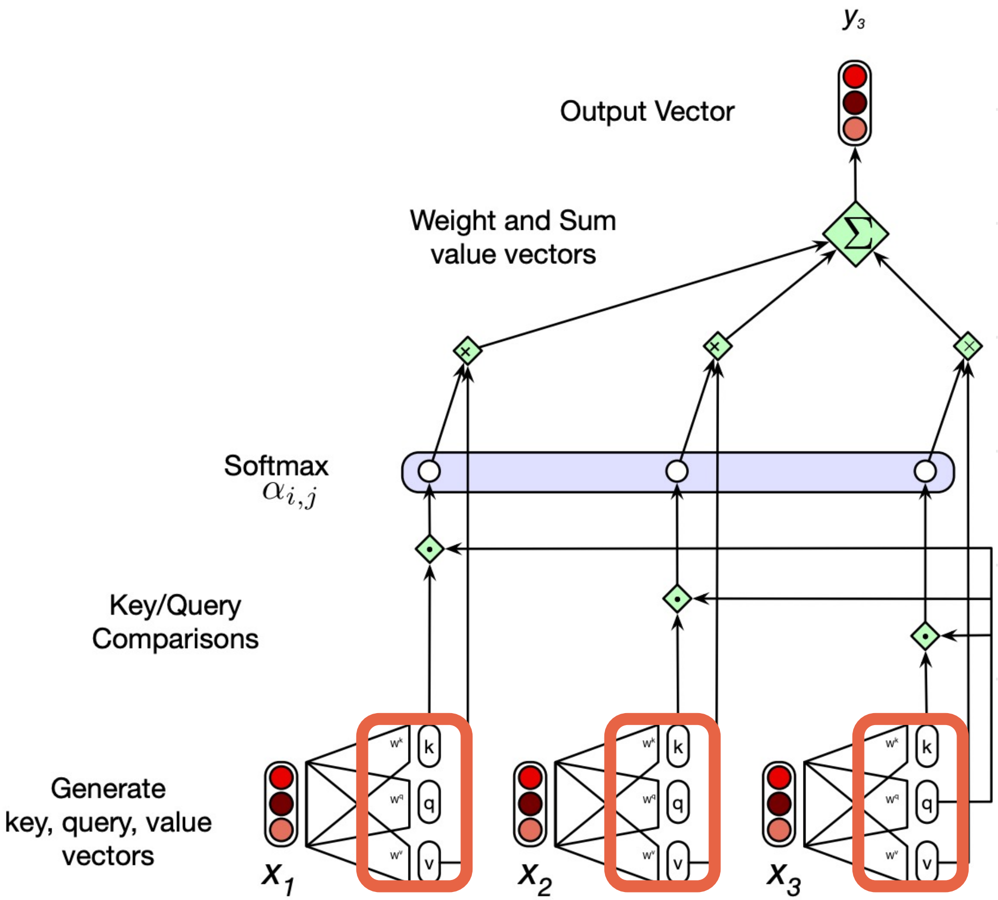


During training, we also **<u>learn weight matrices $W^Q$, $W^K$, and $W^V$,</u>** which we multiply by input **X**.

$$\mathbf{Q} = \mathbf{X}\mathbf{W}^{\mathbf{Q}};\ \ \mathbf{K} = \mathbf{X}\mathbf{W}^{\mathbf{K}};\ \ \mathbf{V} = \mathbf{X}\mathbf{W}^{\mathbf{V}}$$

Learned just like standard weights—by iteratively updating through **back-propagation**.

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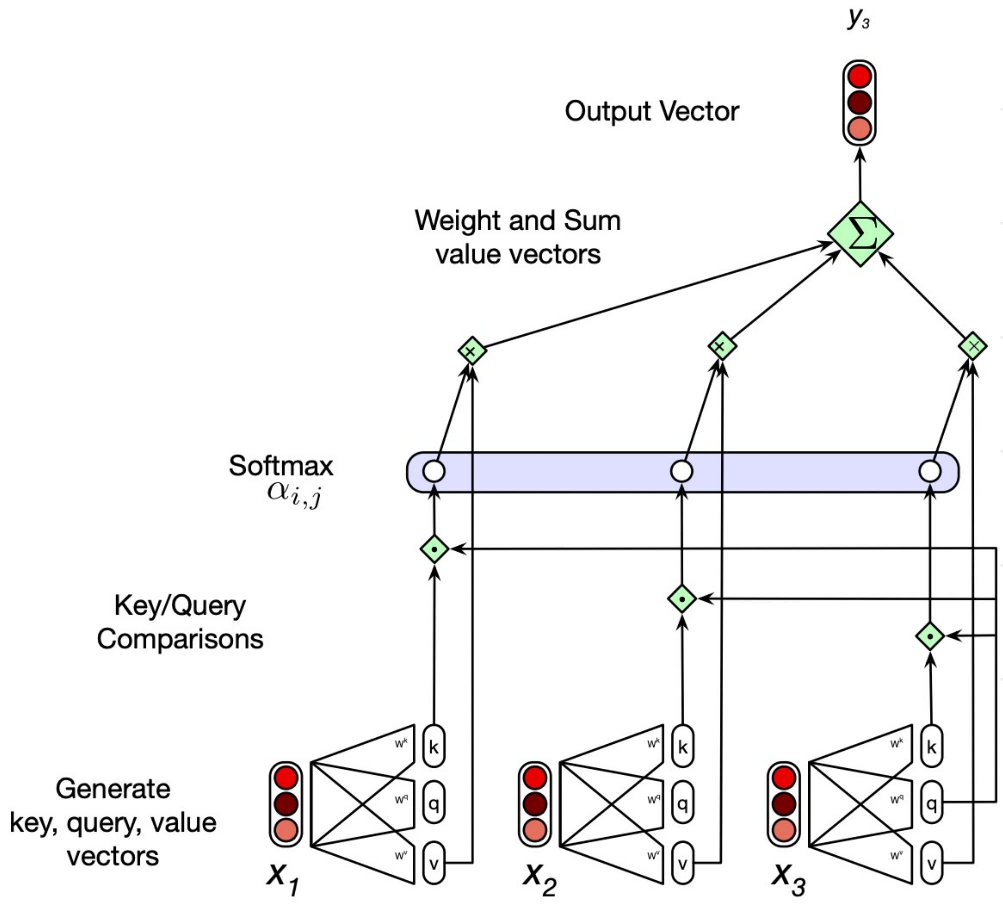
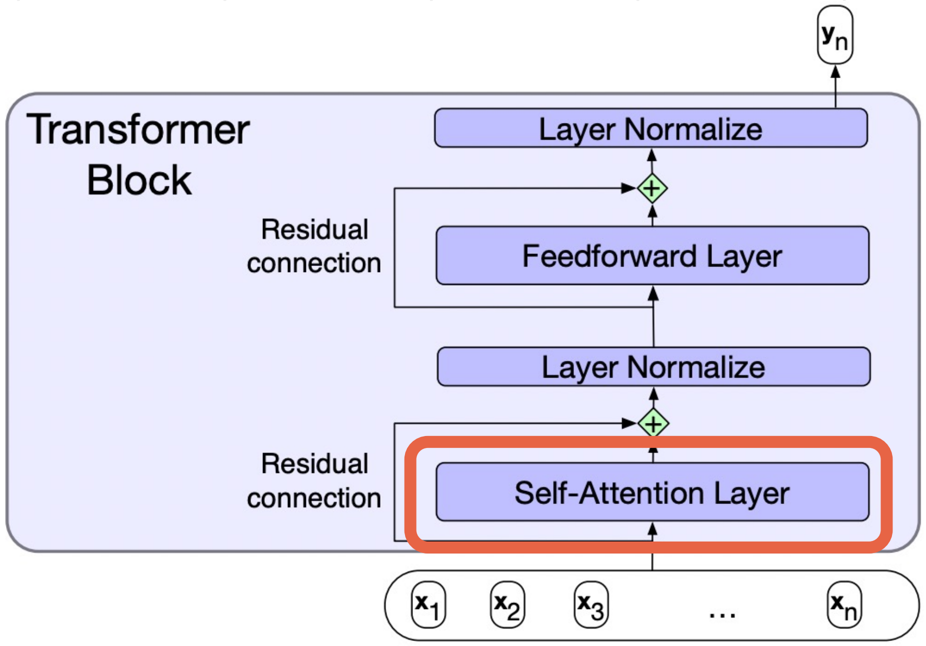
# Self-attention: a closer look




But self-attention is just **one component** of the Transformer…

# The Transformer “block”

A **Transformer** “block” contains a self-attention layer, feed-forward layers, residual connections, and normalizing layers.




Self-attention: used to compute new, context-dependent representations for each token.

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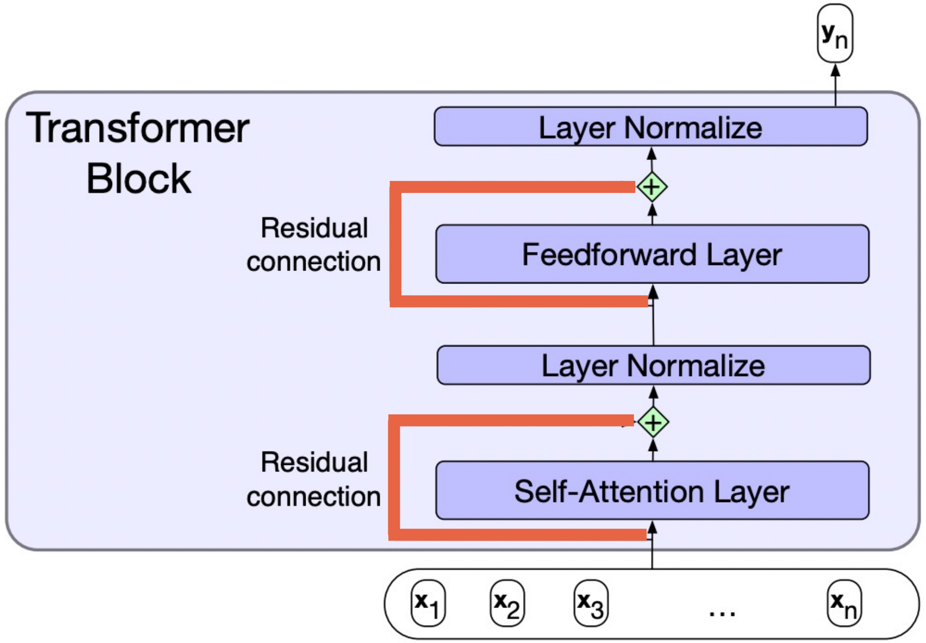


The **"residual connection"** projects directly from a lower layer to a higher layer, without passing through the intermediate layer.

To implement, add a layer's *input* to its *output* before passing it forward.

```
"dog" + Self-Attention("dog")
```

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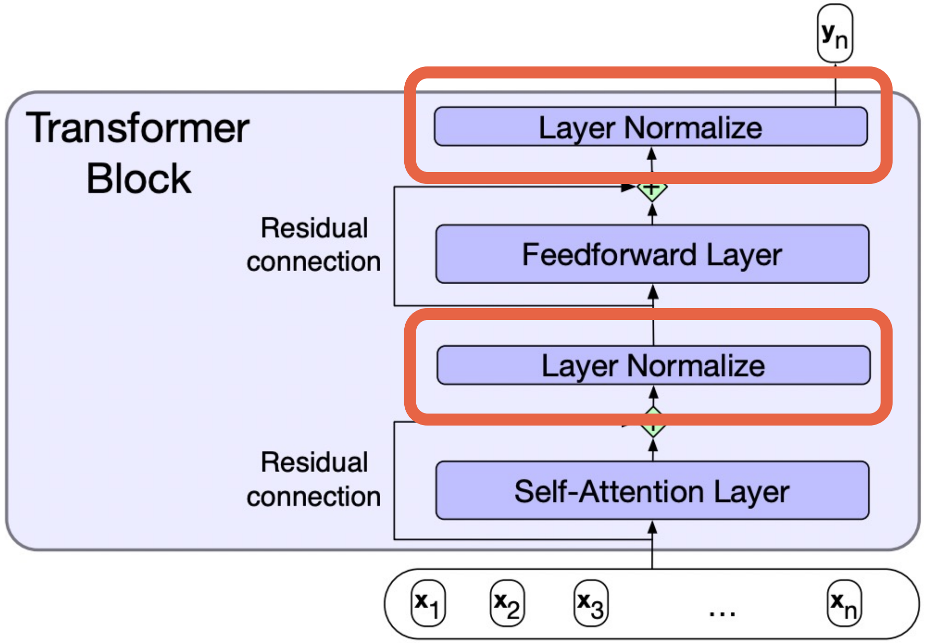


**"Layer normalization"** keeps the values of a hidden layer within a range that facilitates gradient-based training—similar to a *z*-score.

In GPT-2 and GPT-3, this FFN has **two layers**.

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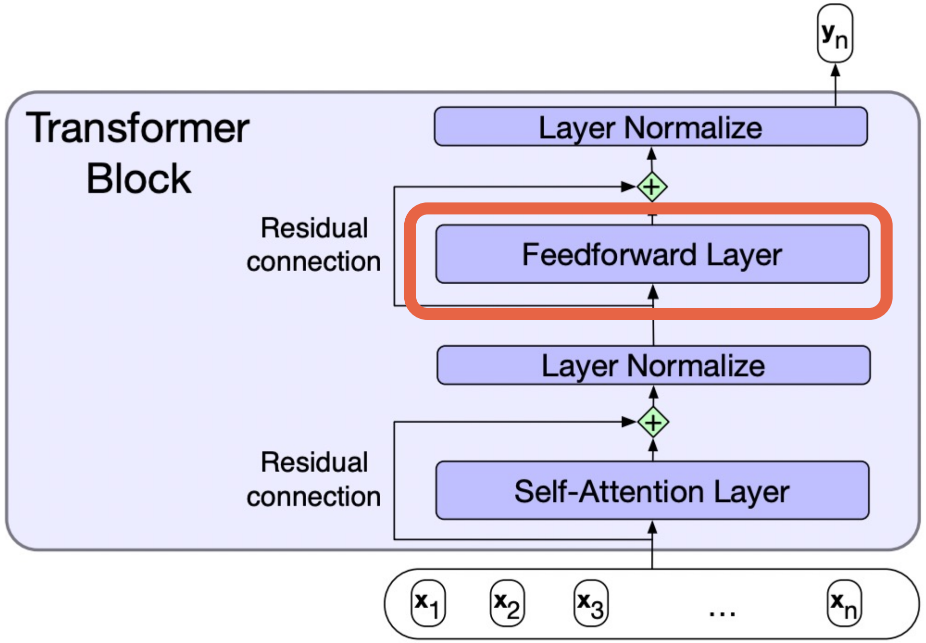
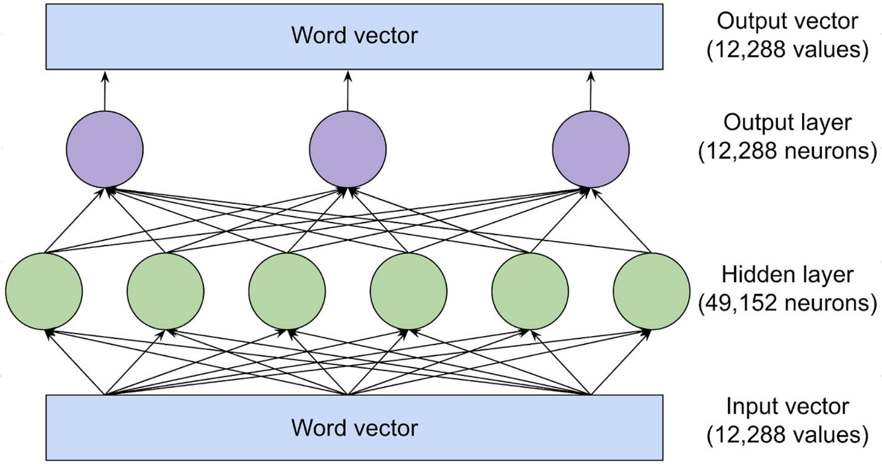



These vectors are then passed to a **feed-forward network**.




Schematic of FFN in GPT-3.

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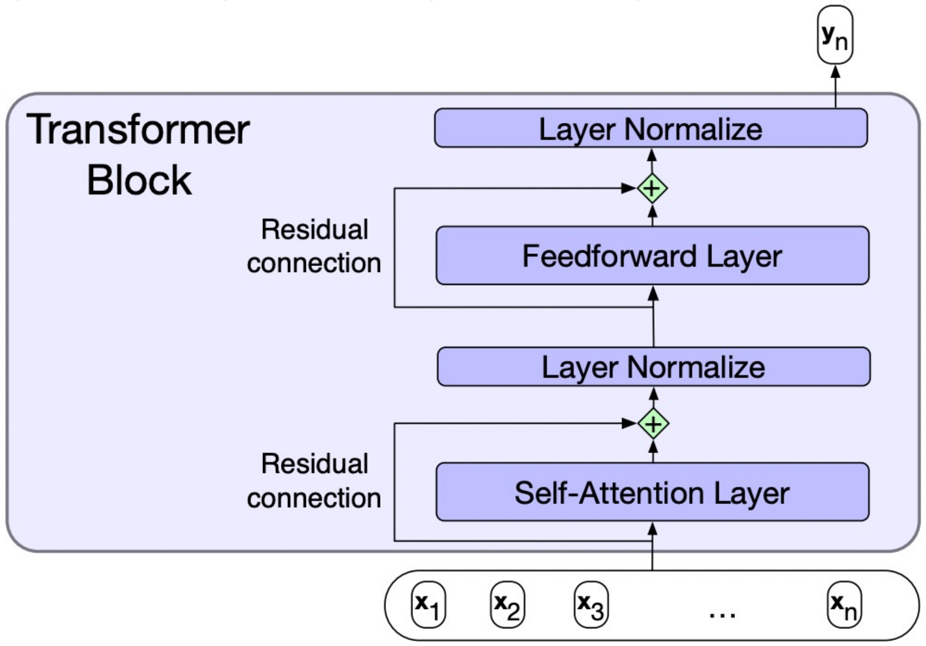


Also called *decoder blocks*.

Models like GPT-2 and GPT-3 have *many* of these!

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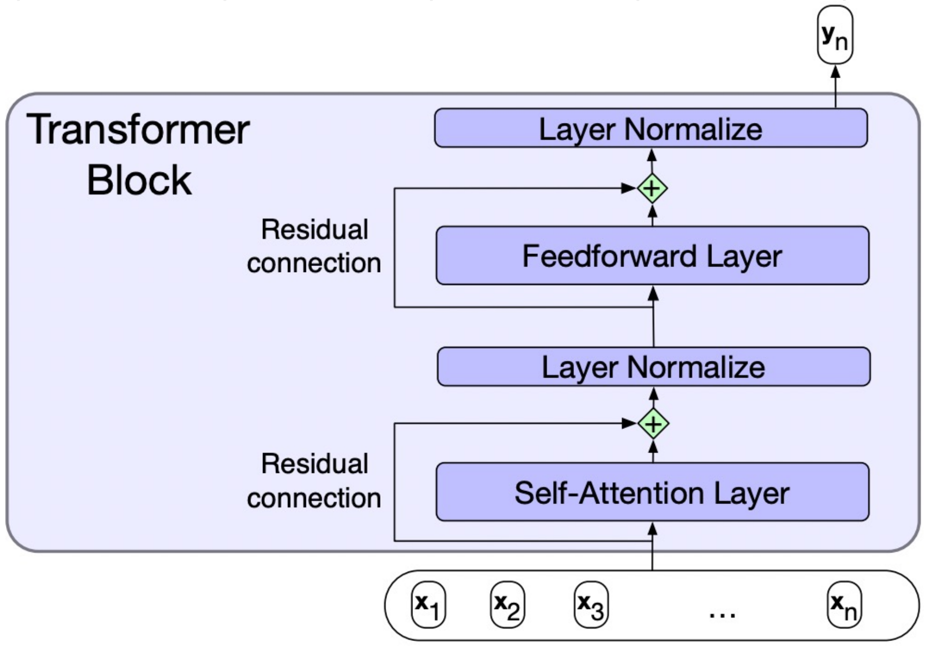


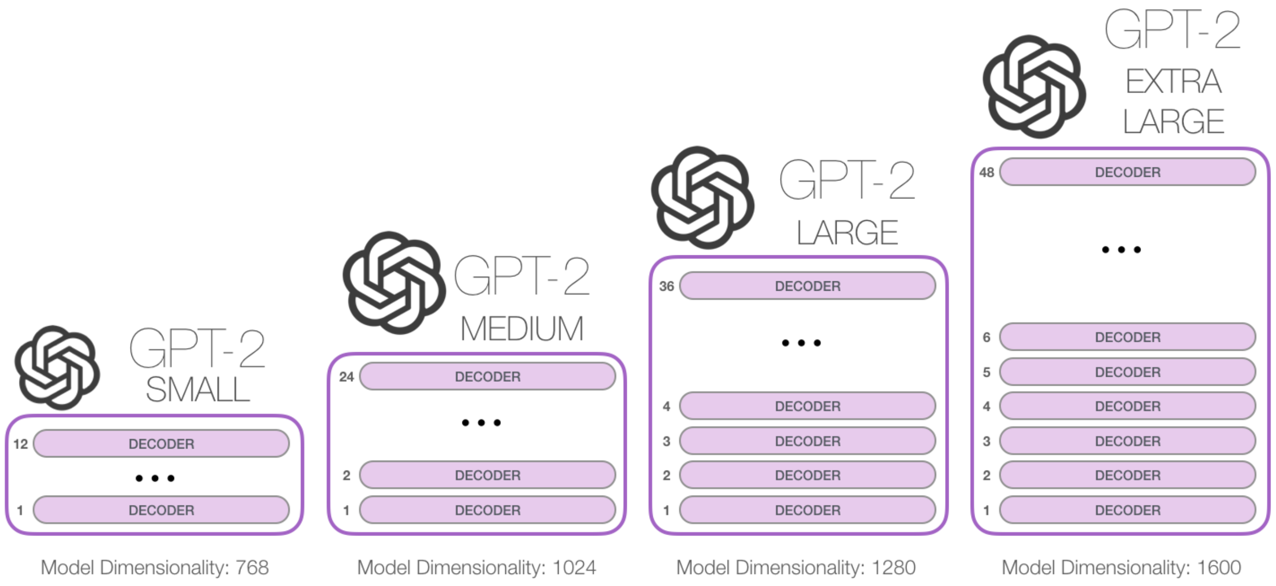

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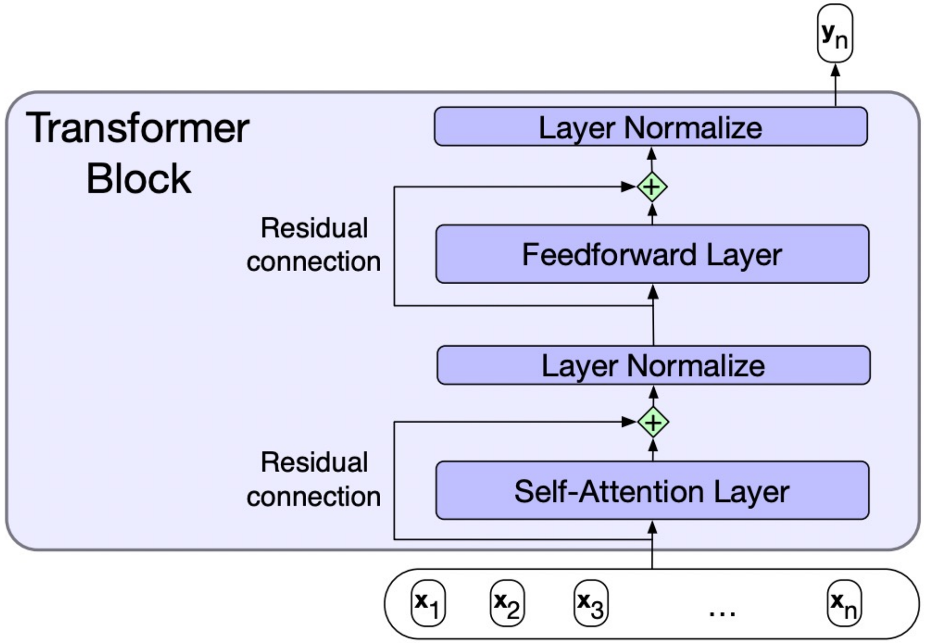
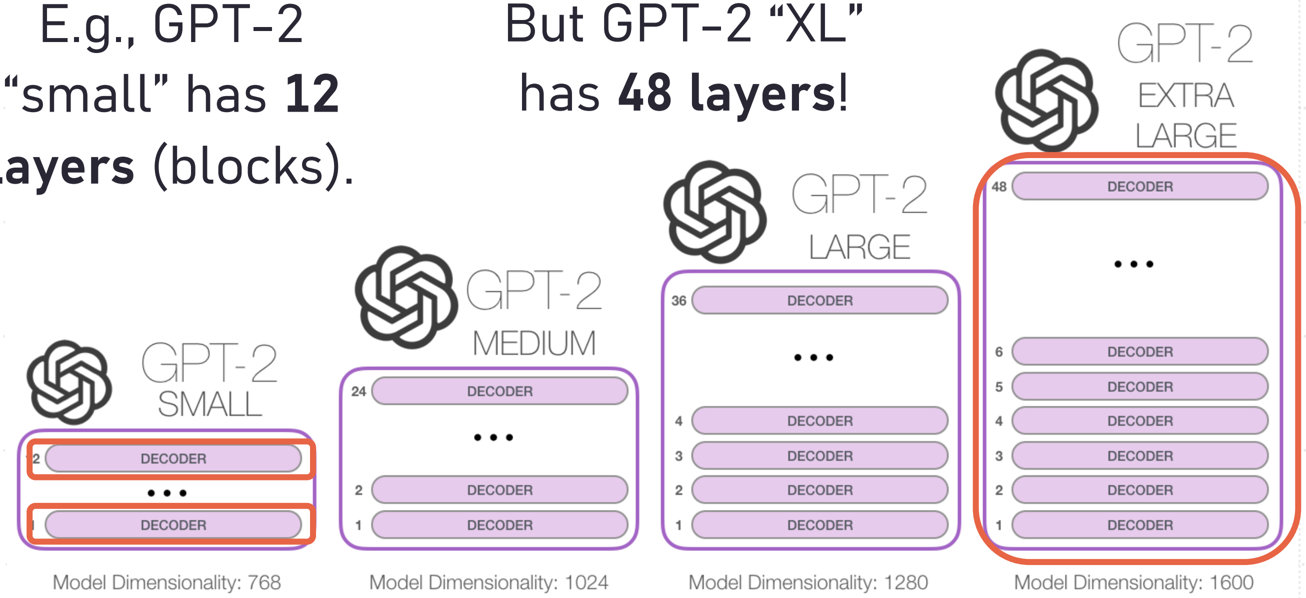



E.g., GPT-2 "small" has **12 layers** (blocks).

But GPT-2 "XL" has **48 layers**!



"RNN + Attention—but throw out the RNN!"

# Introducing transformers

The **Transformer** is a neural network architecture that uses multi-head self-attention, with no recurrent units.

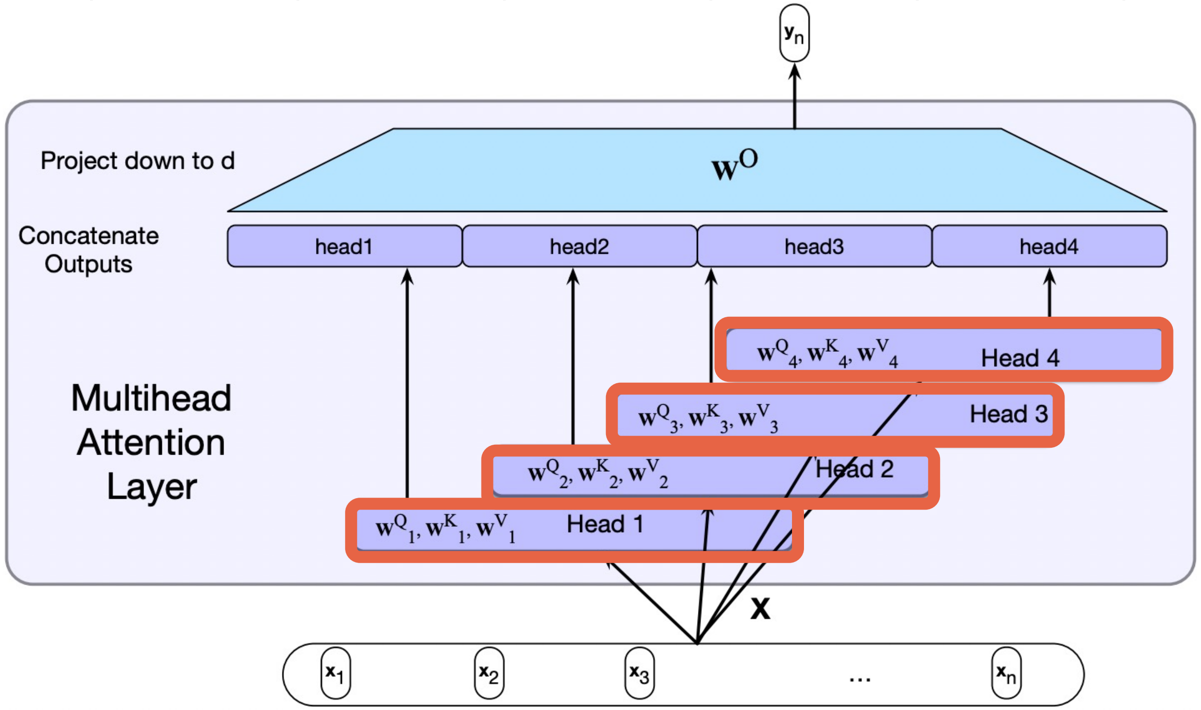
- Use a **fixed context window**.
- No **recurrent connections**.
- Use **self-attention**.
- Have multiple attention "heads" (**multi-head self-attention**).
- Use **positional embeddings**.

We've now covered self-attention— but what's "multi-head" attention?

When we discuss **probing** and **mechanistic interpretability**, we'll talk about research trying to figure out what these heads actually do!

# Multi-head attention

In **multi-head attention**, each layer has multiple attention "heads", each with their own set of learnable weights for producing queries, keys, and values.




Each "head" might learn to track different kinds of relationships.

Over-simplified example:

- Maybe one head tracks syntax.
- Another head tracks proper names.
- Another head tracks events…

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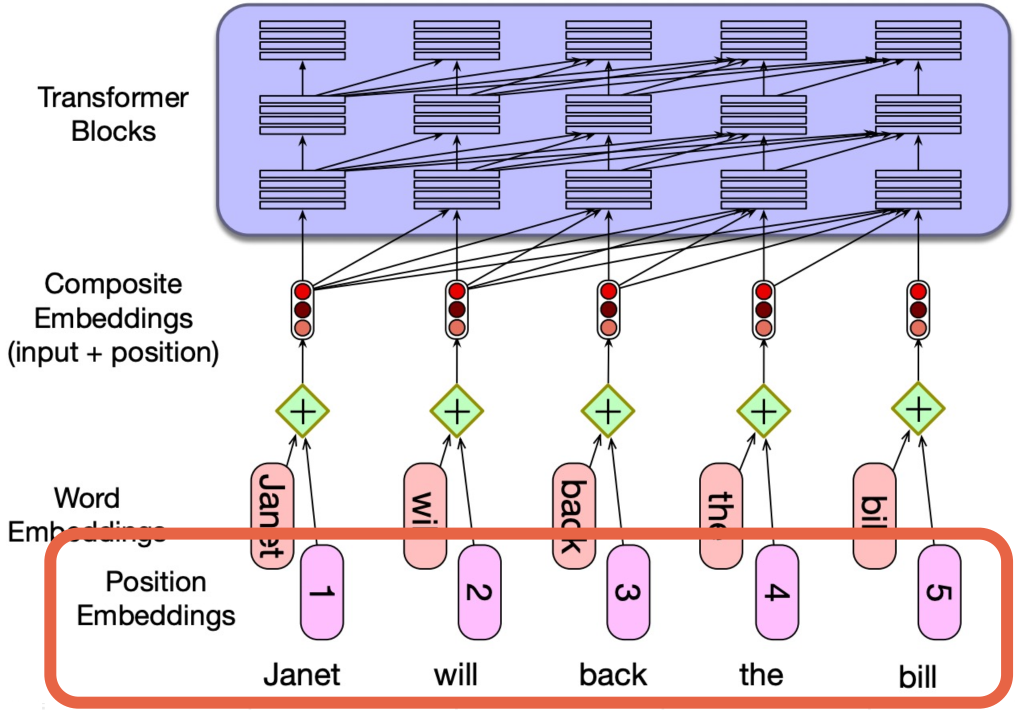
Okay, but what about the **order** of tokens?

With RNNs, order is built into the structure of the network.

Transformers use **positional embeddings** to track order.

# Positional embeddings track order

To represent order, input embeddings are combined with **positional embeddings** specific to each position in a sequence.




To learn, begin with random embeddings representing each "position" in a sequence (1, 2, 3, ...)

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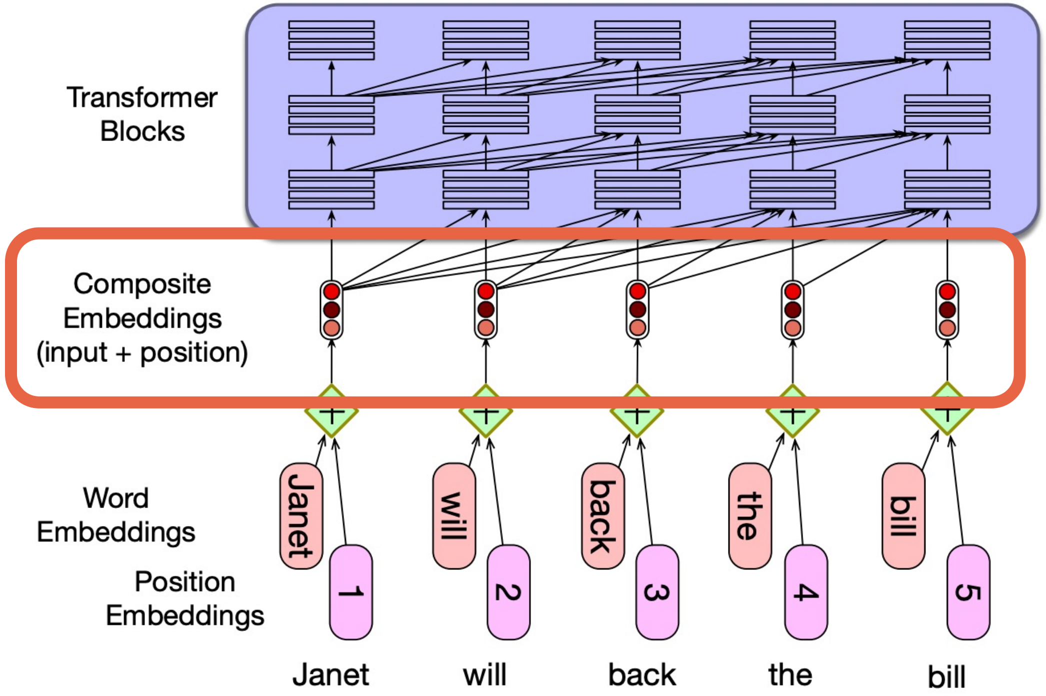


To learn, begin with random embeddings representing each "position" in a sequence (1, 2, 3, …)

Once learned, we add positional embeddings with word embeddings.

Now, composite embeddings reflect both *word* and its *position*.

“RNN + Attention—but throw out the RNN!”

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These are very complicated systems! Still lots to learn about why this architecture works.

One practical benefit is (so far) transformers are easier to train than RNNs.

"RNN + Attention—but throw out the RNN!"

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**GPT** = **G**enerative **P**re-trained **T**ransformer

So what's that "pre-trained" word mean…?

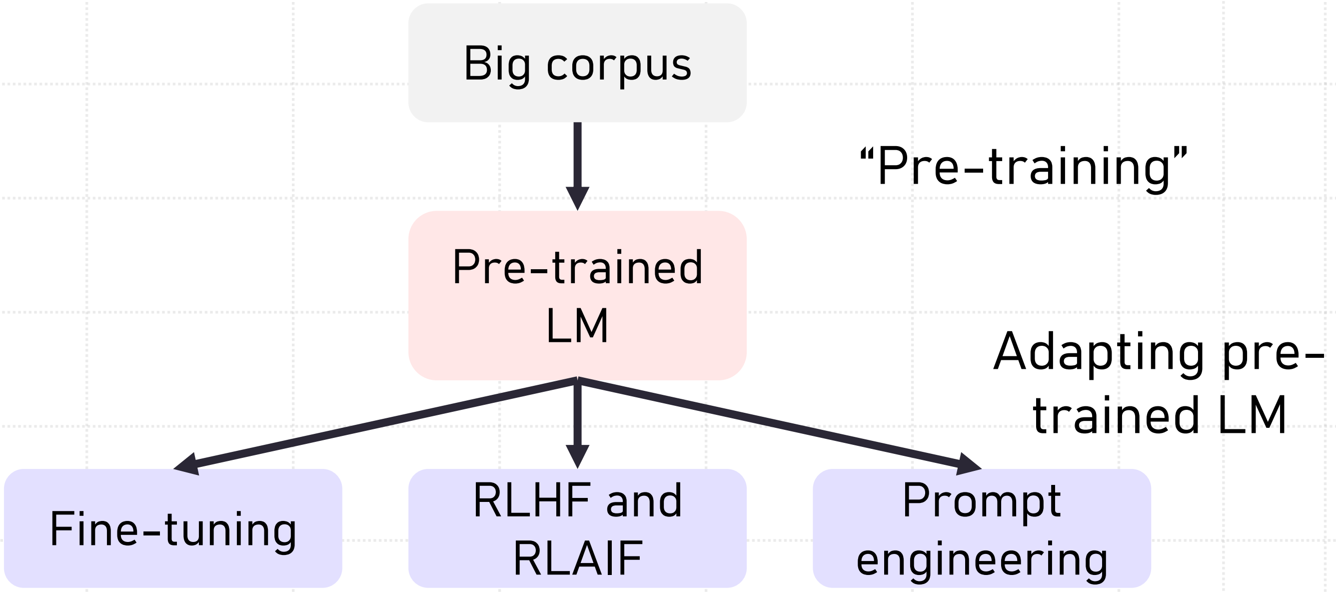
# Lecture plan

- “Attention”: high-level introduction and motivation.
- The transformer architecture—is attention all you need?
- The advent of “pre-trained LLMs”.

# Pre-trained language models

A **pre-trained language model** is a (large) language model that's already been trained on a large corpus using self-supervision.

- "Pre-training" just means training **without a specific end goal in mind** (besides word prediction).
- A "pre-trained" LM can then be **adapted** for specific purposes.
- Practically, it's helpful so we **don't have to train from scratch**!



This is what we'll talk about next time!

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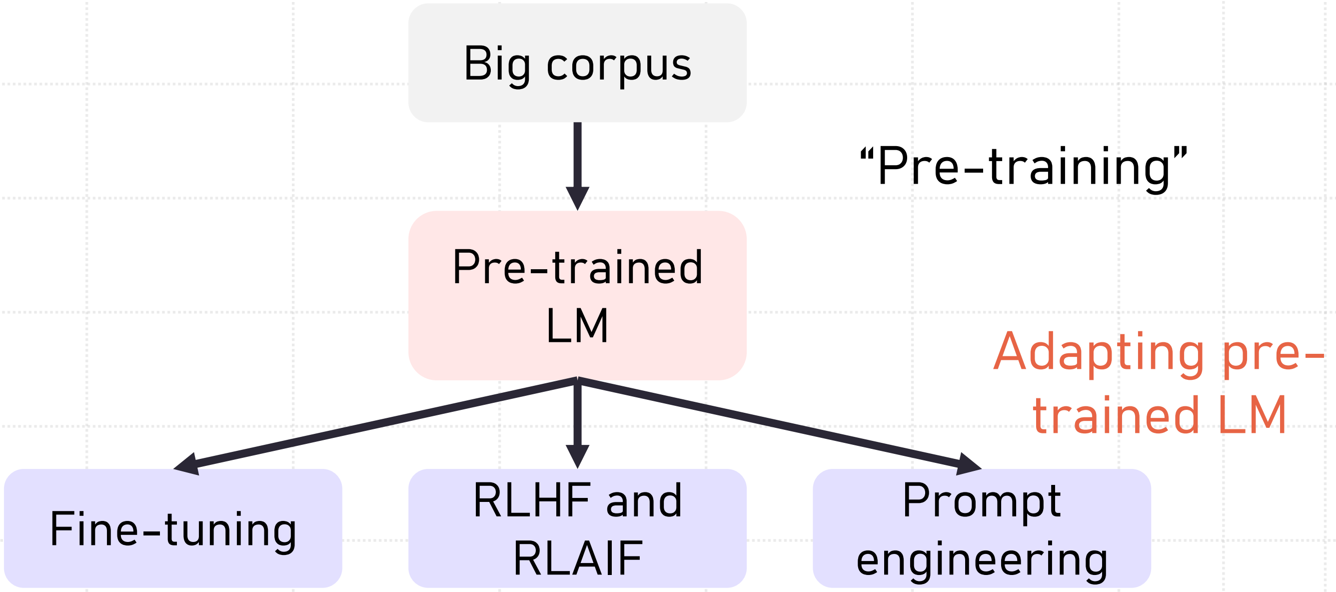

# Summary

- **Self-attention** is a mechanism that allows each word to "look for" other words that are relevant in the input.
- This process creates new **context-dependent vectors** that share relevant information across the words in the input.
- Self-attention a key part part of the **"transformer block"**, which also has other features like a feed-forward network.
- So far, transformers tend to work better than other models like RNNs, and are **easier and faster to train**.
- "**Pre-training**" involves training a model (like a transformer) on a large corpus to learn the "basics" of how language works.